



1H NMR of Organic Compounds 2014

Alexander Yarkov

DVD

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DESCRIPTION

1H NMR of Organic Compounds 2014 is the largest collection of high-quality full-scan ^1H NMR spectral reference data available for reliable identification and can serve as the basis for accurate ^1H NMR prediction. Measured on 300/500MHz instruments, the spectral library contains 157,000 full-scan high-resolution spectra.

Collected and reviewed by Alexander Yarkov, each spectrum in *1H NMR of Organic Compounds 2014* contains carefully reviewed peak assignments, with a corresponding chemical structure and specific measurement and instrument parameters where available. Using proprietary quality assurance measures developed by the author and Wiley, this is the finest and largest collection of ^1H NMR spectra available.

Applications include synthesis confirmation and identification of both "*known unknowns*" (compounds that are contained in the library) and the generation of predicted spectra to match against "*unknown unknowns*" (spectra that can be predicted by training a prediction algorithm on the library and then predicting the spectrum of a new structure for a compound that is not contained in the library). Spectral prediction is constrained only by the chemical diversity of the underlying library, the accuracy of the chemical structures and peak assignments, and the limitations of the spectral prediction algorithm.

Note fields include Name, Source, CSearch ID, Wiley ID, Citation, and Solvent.

Spectra:

- ^1H NMR Spectra: 157,000

- Structures: 157,000
- Compounds: 155,000
- Replicate Spectra: 2,000

Available online on Wiley Spectra Lab, with locally hosted formats available for purchase through ACD/Labs and Mestrelab software.

ABOUT THE AUTHOR

Dr. Alexander Yarkov, born in 1954 in Russia, attended Lomonosov Moscow State University in the department of chemistry from 1971 to 1976. He then continued as a postgraduate student in the physical chemistry department, working in a molecular spectroscopy laboratory until 1979. In 1982, he was a candidate of chemistry for Moscow State University. Dr. Yarkov is now the senior scientist for the Applied Spectroscopy Laboratory at the Institute of Physiologically Active Compounds at the Russian Academy of Science. His research areas of interest include molecular spectroscopy, NMR spectroscopy, mass spectroscopy, identification of chemicals using spectral databases, and QSAR.

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